The NIST Chemistry WebBook:
A Chemical Data Resource on the Internet

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The NIST Chemistry WebBook (http://webbook.nist.gov) is an Internet site that provides access to chemical and physical property data from NIST and other sources. The site was established in 1996 and has grown to encompass a wide variety of thermochemical, ion energetics, solubility and spectroscopic data. Available data include both data from the NIST and outside contributors. Where appropriate, citations to the literature are provided along with the data. In many cases comments and auxiliary data accompany the data from the researchers who collected the data.

A number of facilities are provided for searching for chemical data. These include chemical formula, name, and structure searches. Searches based on physical properties are also provided. Search-able physical properties include ion energetics properties, electronic and vibrational spectra, and molecular weight.

A wide range of physical and chemical property data is available from the site. Thermodynamic data include properties for single phases, phase transitions, and reactions. Several large databases of ion energetics data are incorporated in the site, including data for simple ions and ion clusters. Spectral data include gas phase IR spectra, UV/Vis spectra, mass spectra. Vibrational and electronic spectra are available for a number of transient and stable species. The site also includes a collection of constants of diatomic molecules and a collection of Henry's law constants.

In addition to data tables, the site includes several special features. Interactive models for state properties are provided for 16 common fluids. Dynamic graphical displays are provided for several types data, including IR mass and UV/Vis spectra, and several thermodynamic quantities. A simple drawing applet allows users with Java capable browsers to draw and submit chemical structures for searches.

This exhibit will include demonstrations of the web site and tips on using it effectively.